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ME469: Nalu Overview

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U.S. DEPARTMENT OF
ENERGY

NNSA

Lecture Objectives

- Nalu Technology Origination: Advanced Simulation and Computing project (NNSA)
- Beyond the 32-bit Limit
- Supported Physics
- Supported Numerics
- Low- and High-order
- Moving Mesh (Sliding and Overset)
- Multiphysics
  - Fluid Structure Interaction
  - Conjugate Heat Transfer (CHT)
  - Participating Media Radiation
  - Examples

Core Technology Provided to Nalu Origination: Advanced Simulation and Computing Sierra/Fuego

- Use-case characterized by a highly sooting, turbulent, reacting flow with Participating Media Radiation (PMR), Conjugate Heat Transfer (CHT), and propellant multi-physics coupling


- Complex geometry has driven a generalized, hybrid unstructured discretization approach supporting Hex8, Tet4, Wedge6, and Pyramid5 elements in addition to promotion of Hex8 to Hex27, and Tet4 to Tet10

Goal: Beyond 32-bit Computing

- Circa 2013, many scientific production codes were limited to 32-bit

- Therefore, maximum simulation size for entities, e.g., node, edge, face, element, etc., was ~2.2 billion

- Next Generation Platforms were advocated to overcome poor MPI scaling and power needs to support Exascale computing (10^{18} floating point operations/second)
  - Platform architectures, at that point, were not not yet known (still evolving)

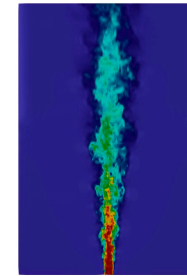+ ASC Investments

( )
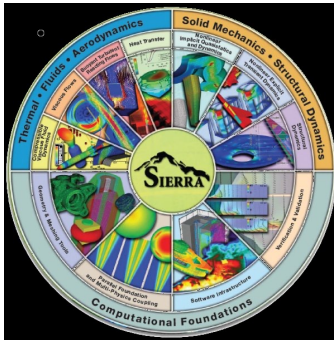
Sierra Toolkit/Trilinos (open-source)
MPI+X parallelism
Support for new architectures

Developed Open-Source BSD-clause 3 Distribution Policy
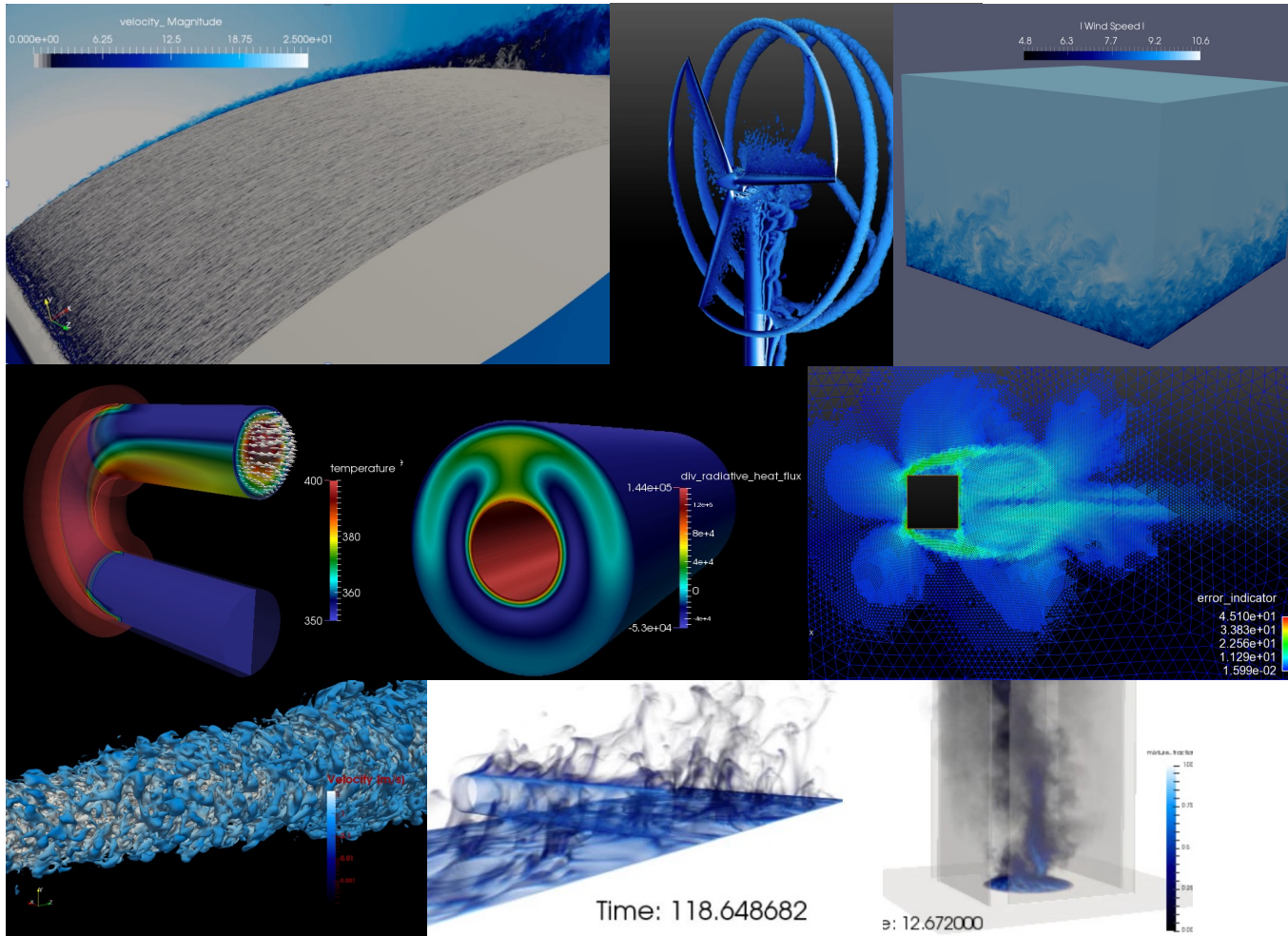
- Philosophy: Open-source collaborations
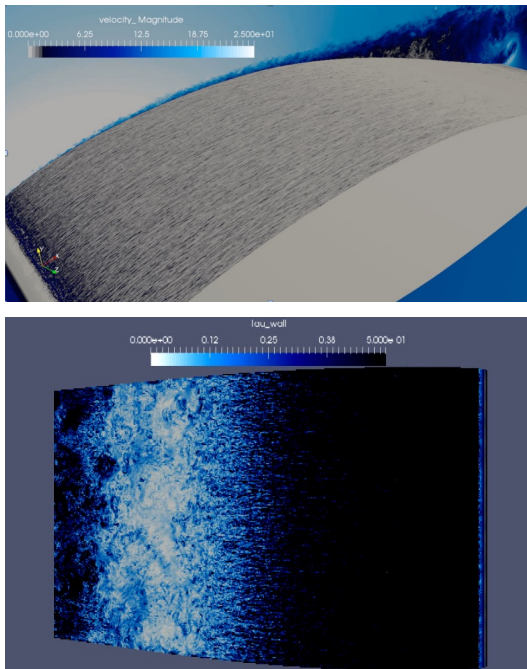

https://github.com/NaluCFD
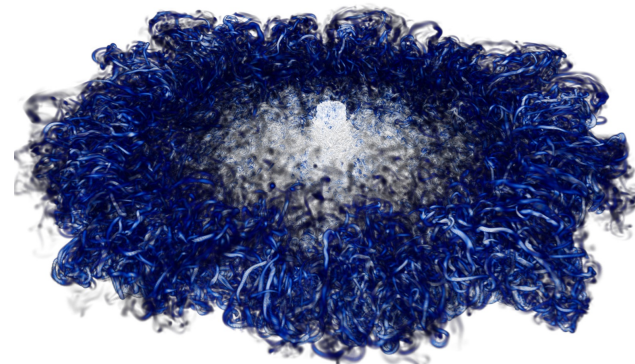
Supported Physics: DNS and LES (even RANS)

A Note on High Performance Computing

Sandia (and Stanford) are committed to High Performance Computing (HPC) to support is science and engineering objectives: Exercised herein

O(2) billion DNS impinging jet

O(6) billion wind energy application
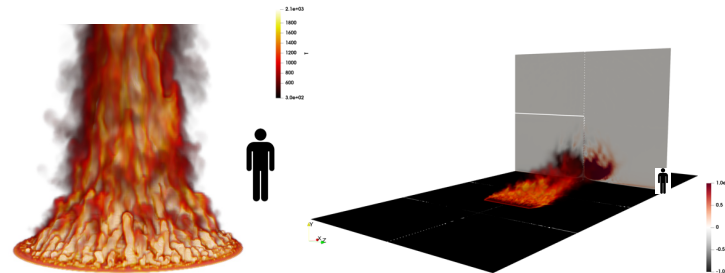
O(200) million multi-physics fire

Nalu Timeline/History

- By CFD standards, this is a relatively new code base

Sierra/Nalu — SNL License →

Open-source BSD License (2014) ↓

Github Nalu — Active academic partners → .... etc

ECP ExaWind (2018) ↓

Github Nalu-Wind — Open-source: SNL, NREL, ORNL, UT joint copyright
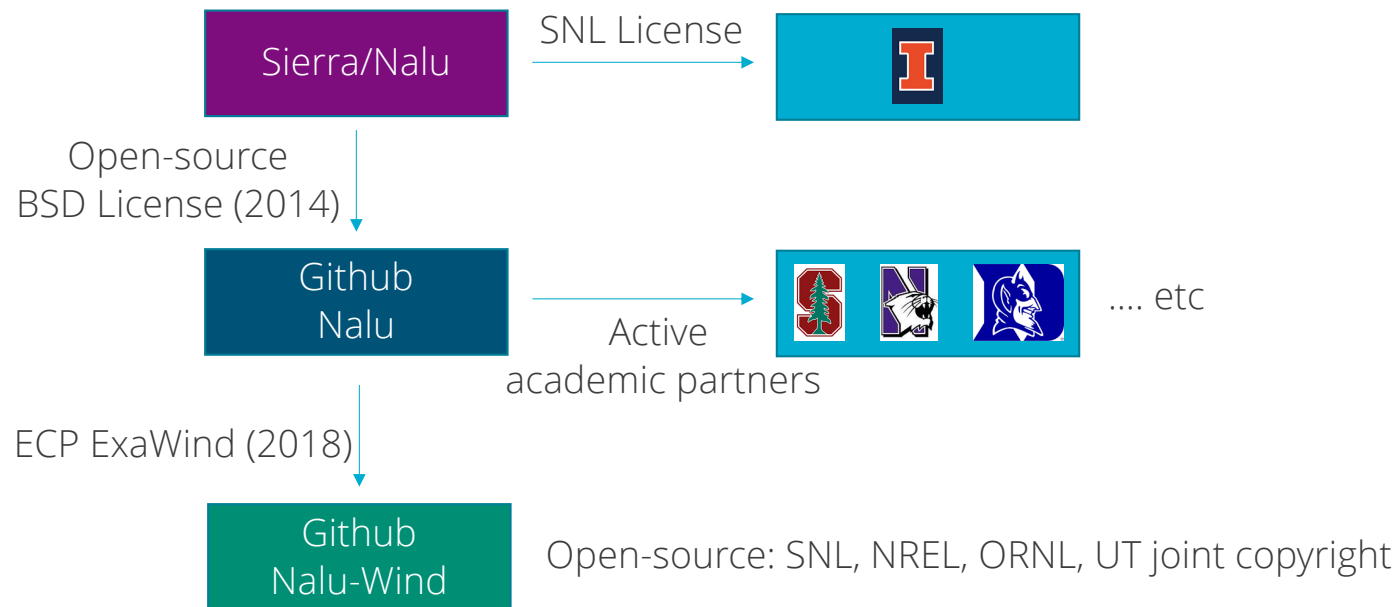
Several Multi-physics Flow Examples From Nalu

Cylinder in cross flow

Helium plume (low-/high-order)
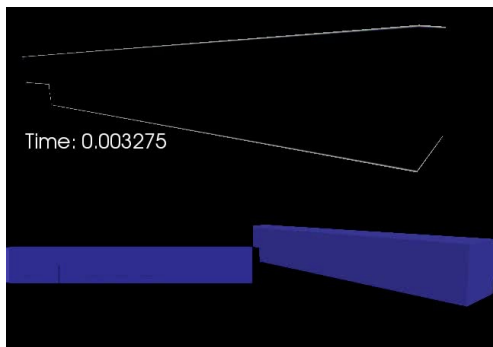
Heated backstep
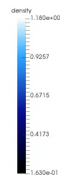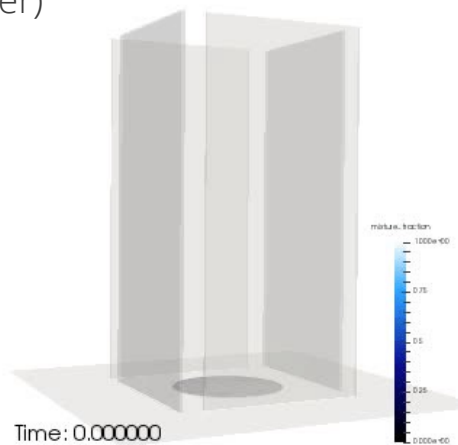
Whirling behavior
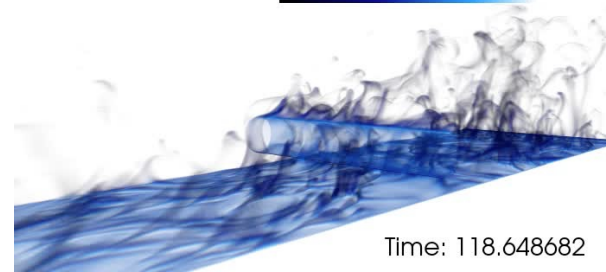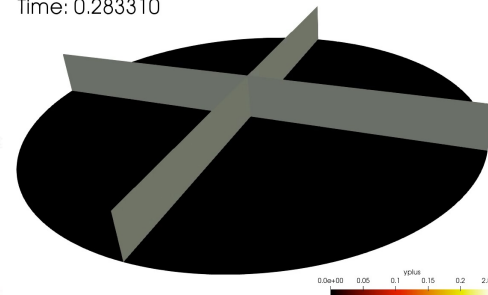
Impinging Jet DNS

Nalu Abstractions: Polymorphic and Input File-Driven

Time Integration

Nonlinear Coupling

Realm A

Realm B

1 to many Interior algorithms

1 to many Interior algorithms

1 to many boundary algorithms

1 to many boundary algorithms

Transfer

Operator-split multi-physics
Conjugate heat transfer coupling
- Fluids Realm
- Heat Conduction Realm
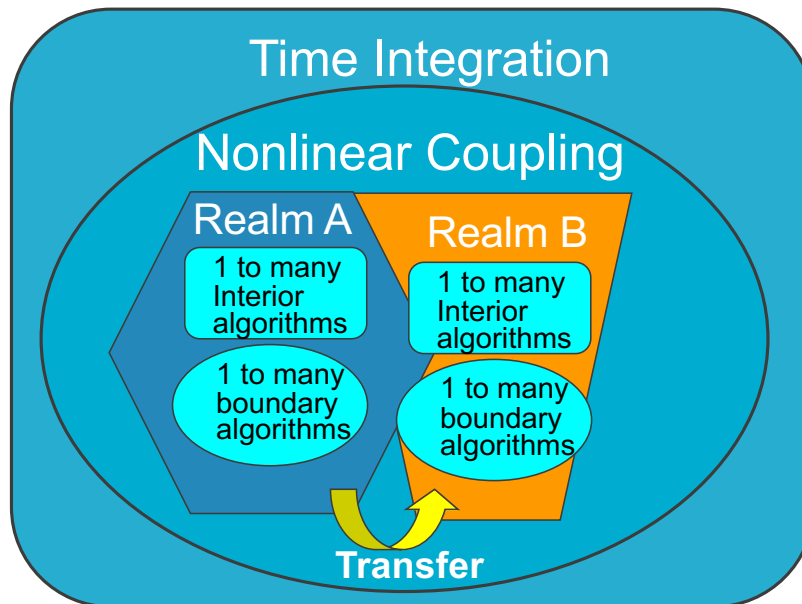
- *Realm* specifications define the physics and desired boundary conditions

- Pre-defined *EquationSystems* (segregated or monolithic)
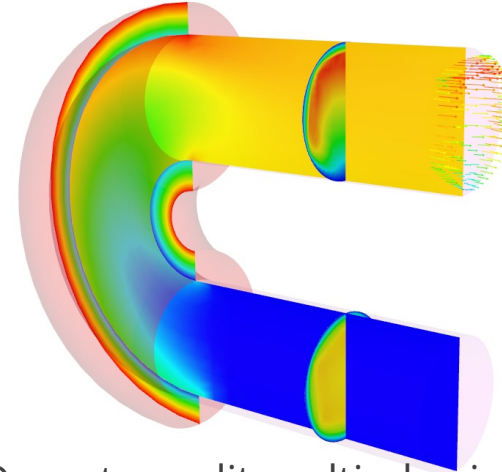
Operator-split multi-physics:

- Conjugate heat transfer coupling
  - Fluids and solid Realm

Essential Attributes of a CFD Simulation

- Mapping from Real World, to Conceptual Model, and, finally, a Computer Model (given an underlying PDE discretization approach)

Mesh

Input File(s)
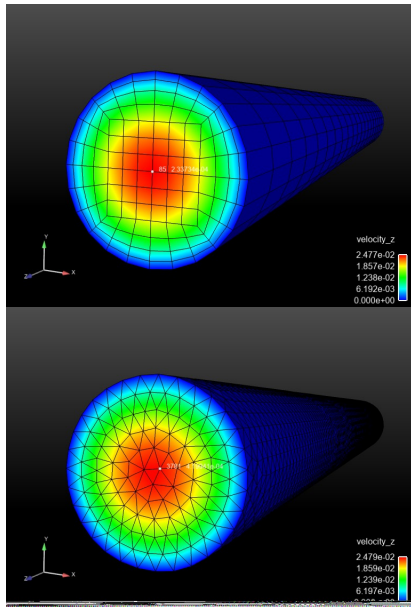
mesh: my_mesh.g
euations: my_equations

- inflow_boundary_condition: bc_left
    target_name: Inflow
        velocity: [1.0,0.0
        mixture_fractio

Hex8

Tet4

launch remotely

launch locally
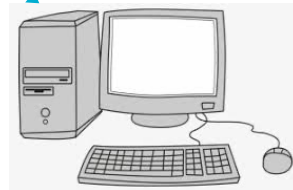
Remote Viz

output.log
output.e.32.*
output.rst.32.*

ParaView

>scp output.e.32.* /to/my/local/disk

30K View: Anatomy of a Nalu Input File:YAML-based

Simulation:

linear_solvers: ←—————— Specification of sparse Trilinos-based precond/solver

transfers: ←—————— Data transfer for multi-physics coupling

realms:

YAML enforces strict spacing and ordering

  - name: realm_heatCond

    boundary_conditions:
    - wall_boundary_condition: bc_exposed

    solution_options:
    initial_conditions:
    material_properties:
    equation_systems:

Physics definitions

      systems:
        - HeatConduction:

    output:
    restart:

  - name: realm_fluids

TimeIntegrators: ←—————— Time integration, e.g., BE, BDF2

High-Level Elements of an Input File

systems:

   - LowMachEOM:
      name: myLowMach

   - MixtureFraction:
      name: myZ

initial_conditions:

   - constant: ic_1
      target_name: [block_1, ...]
      value:
       pressure: 0
       velocity: [0.5,0.0]
       mixture_fraction: 0.0

boundary_conditions:

   - inflow_boundary_condition: bc_left_inflow
   - wall_boundary_condition: bc_front_wall
   - open_boundary_condition: bc_right_open
   - symmetry_boundary_condition: bc_top
   - nonconformal_boundary_condition: bc_nc

material_properties:

target_name: block_1

specifications:

   - name: density
     type: constant
     value: 1.0

   - name: viscosity
     type: constant
     value: 1.8e-5

material_properties:

target_name: block_1

specifications:

   - name: density
     type: ideal_gas

   - name: viscosity
     type: polynomial
     coefficient_declaration:

   - inflow_boundary_condition: bc_left
     target_name: surface_1
     inflow_user_data:
      velocity: [0.5,0.0,0.0]
      mixture_fraction: 0.0

   - wall_boundary_condition: bc_back
     target_name: surface_7
     wall_user_data:
      user_function_name:
       velocity: wind_energy
      user_function_string_parameters:
       velocity: [mmTop_ss7]
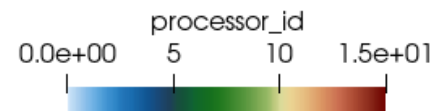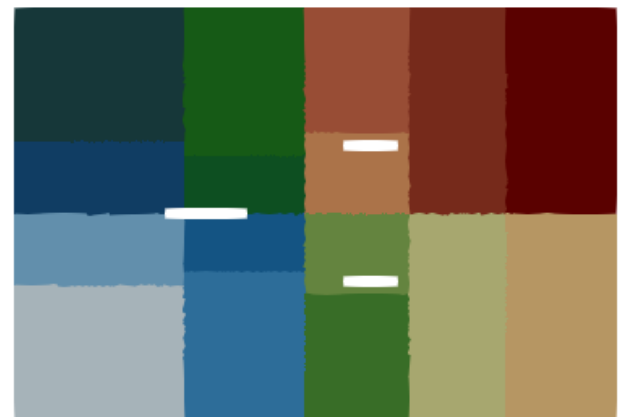   mixture_fraction: 1.0

A Note on Parallel Decomposition

- Decomposing the mesh into small subsets and operating on these subsets in parallel provides a methodology for increased simulation time
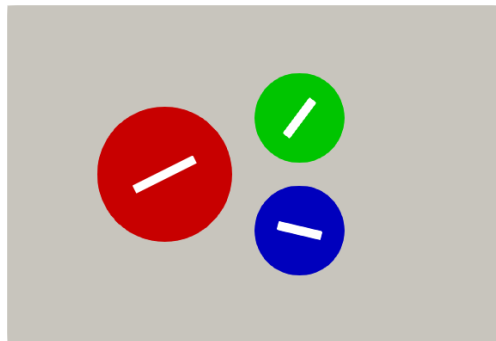
Colored by block ID

Colored by core count (= 1) One mpi rank.

16 MPI ranks = 16x faster (hopefully)

processor_id

0.0e+00   5   10   1.5e+01

How to Run in Parallel: Mesh Decomposition

- Given a mesh, mesh.g and myInputFile.i, if one desires to run on, e.g., 16 core case:
  1. Use pre-processing "decomposition" tools (Trilinos/install/bin)
  2. In-situ decomposition

>/path/to/decomp –j {np} {meshName}
>mesh.g.16.00, mesh.g.16.01, .., mesh.g.16.15

1:   - name: realmFluids
       mesh: mesh/myMesh.g
       ~~automatic_decomposition_type: rcb~~

myMesh.g

2: - name: realmFluids
      mesh: mesh/myMesh.g
   automatic_decomposition_type: rcb

processor_id
0.0e+00   5   10   1.5e+01
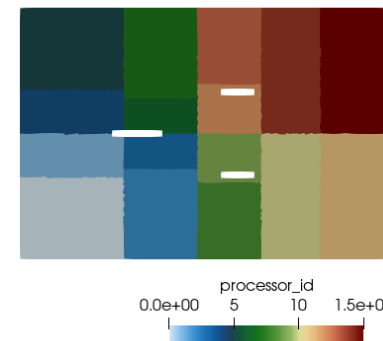
>mpirun --np 16 /naluPath/naluX -i input.i &

>results.e.16.00, results.e.16.01, .., results.e.16.15
>input.log

A Note on Divergence

- Whether by design or poor code usage, solution results from CFD analysis for complex applications may diverge. How do I know?

- Non-finite residuals, i.e., not-a-number:"nan" (either linear or non-linear),
  - const double norm = 0.0;
  - const double flux = rho*u*A/norm;

- What if the simulation runs, however, results look very wrong? Typical causes?
  - Bad initial condition that drives nonlinear solution to diverge
  - Too large of an initial time step
  - Poor stabilization, numerical parameters, etc.
  - Poor time integration
  - Ph.D. from ICME explaining why...
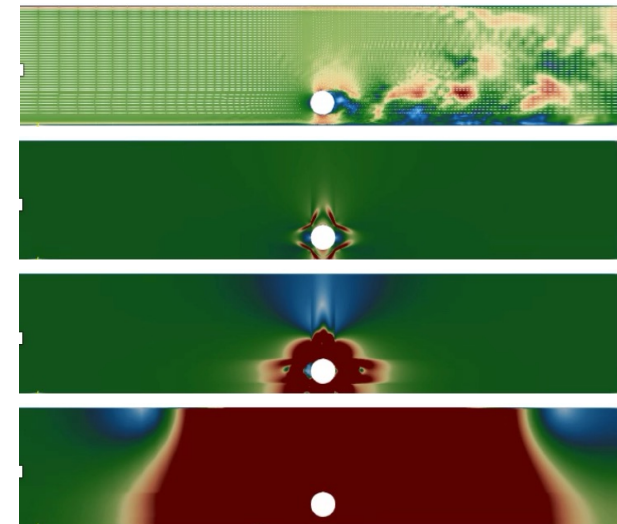
EBVC flow-past 2D cylinder
Top: +NOC
Bottom se: -NOC

Test Case Input Files

- Input files are part of the Nalu regression test suite: Nalu/reg_test/test_files
- Mesh files are found under: Nalu/reg_test/mesh
- Formally, /mesh is a git submodule

Test Cases Highlighted:
1. Nalu/reg_tests/test_files/dgNonConformalThreeBlade
2. Nalu/reg_tests/test_files/fluidsPmrChtPeriodic

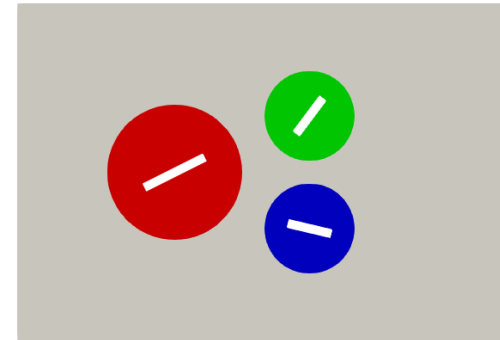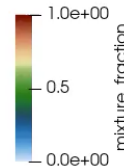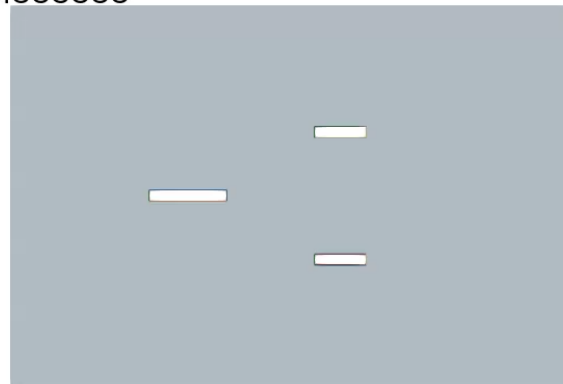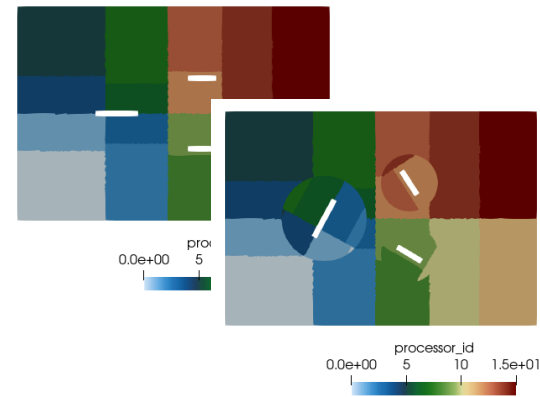Resource: https://nalu.readthedocs.io/en/latest/source/theory/index.html

Nalu/reg_tests/test_files/dgNonConformalThreeBlade

- Physics:
  - Flow past rotating square blades (Re = 10,000)
- Models
  - Newtonian fluid (air) with constant properties
- Boundary Conditions
  - Inflow, open, symmetry, DG/CVFEM interface

Domino, JCP, 2018

Time: 0.000000

>mpirun --np 4 /naluPath/naluX -i dgNonConformalThreeBlade.i &

Nalu/reg_tests/test_files/dgNonConformalThreeBlade

γ_i for BDF2

$U\Delta t / \Delta x$

$\rho \cup L / \mu$

Nonlinear iterations

Equations

Review

```
Time Step Count: 43 Current Time: 0.108355
 dtN: 0.002285 dtNm1: 0.00228982 gammas: 1.49947 -1.99789 0.498422
 Volume  0.818029 min: 1.34303e-06 max: 7.25544e-05
 Max Courant: 2.00422 Max Reynolds: 233.316 (realm_1)
    Realm Nonlinear Iteration: 1/1

realm_1::advance_time_step()
NLI    Name            Linear Iter     Linear Res      NLinear Res    Scaled NLR
---    ----            -----------     ----------      -----------    ----------
1/2    Equation System Iteration
 1/1       myLowMach
           MomentumEQS            5      1.36481e-07    0.000150157           1
           ContinuityEQS         10      9.02089e-07    0.000591053           1
           PNGradPEQS            28      2.69559e-09    1.25557e-06           1
           PNGradUEQS            30      6.93157e-09    3.99347e-06           1
 1/1          myZ
           MixtureFractionEQS     5      7.91662e-09    7.70262e-06           1
           PNGradZEQS            14      3.76375e-09    3.75761e-06           1
2/2    Equation System Iteration
 1/1       myLowMach
           MomentumEQS            5      3.54267e-09    1.77926e-06     0.0118493
           ContinuityEQS          9      6.32285e-07    0.000379046      0.641307
           PNGradPEQS            26       2.3035e-09    1.11406e-06      0.887296
           PNGradUEQS            26       5.6359e-10    3.39699e-07     0.0850636
 1/1          myZ
           MixtureFractionEQS     4      3.36865e-09    1.60783e-06      0.208738
mixFrac clipped (-) 14294 times; min: -0.0414158
mixFrac clipped (+) 2 times; max: 1.03823
           PNGradZEQS            18      1.32816e-10     6.6934e-08     0.0178129
Mass Balance Review:
Density accumulation: 0
Integrated inflow:     -0.375
Integrated open:       0.3749994376540416
Total mass closure:    -5.62346e-07
Mean System Norm: 6.404895358841074e-05 43 0.108355█
```
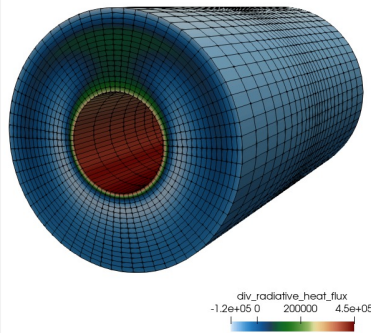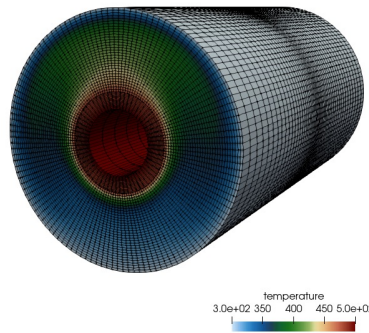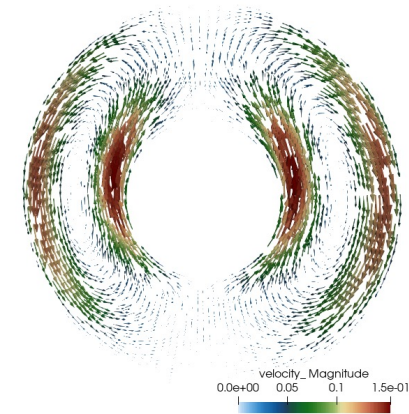
Nalu/reg_tests/test_files/fluidsPmrChtPeriodic

- Physics:
  - Uniformly emitting/absorbing participating media radiation (PMR) conjugate heat transfer (CHT) with buoyancy

- Models:
  - Newtonian fluid (air): ideal gas

- Boundary Conditions:
  - Wall, periodic
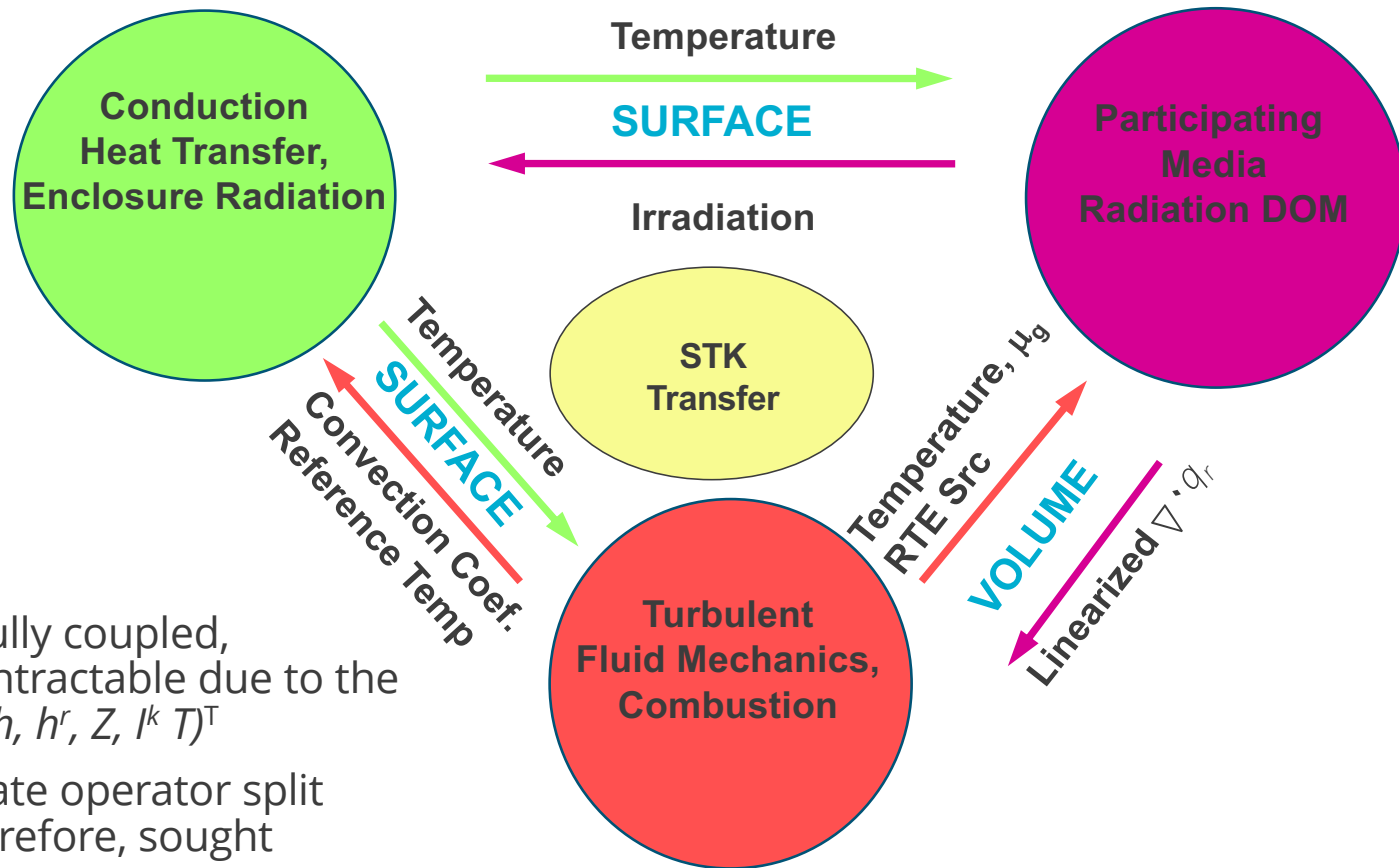

velocity_ Magnitude
0.0e+00   0.05   0.1   1.5e-01

Stark#, cond/rad
$Sk = \lambda \, \mu \, / \, \sigma \, T_i^3 \sim 0.4$

Rayleigh#, $\tau^{ThermalDiff} / \tau^{Conv}$
$Ra = g \, \beta \, (T_i - T_o) \, L \, / \, Pr \, \alpha^2 \sim 2e6$

temperature
3.0e+02 350   400   450 5.0e+02

div_radiative_heat_flux
-1.2e+05 0   200000   4.5e+05

>mpirun --np 8 /naluPath/naluX -i fluidsPmrChtPeriodic.i &

Nalu/reg_tests/test_files/fluidsPmrChtPeriodic

- Monolithic, i.e., fully coupled, approaches are intractable due to the size of $(u, v, w, p, h, h^r, Z, I^k T)^T$

- Stable and accurate operator split methods are, therefore, sought
  - See Domino et al., *AIAA*, 2007

Break-out Example Using Paraview

- Live demo